Top 10 scientific algorithms

Reference:

Science, Vol. 287, No. 5454, p. 799, February 2000

Computing in Science & Engineering. **(*January*, 2000).**

Heros of Algorithms

Euclid

Al-Khwarizmi

Hilbert

Alan M.Turing

History

– **The word algorithm is derived from the name of Abu Ja'far Muhammad ibn Musa al-Khwarizmi, a 9th-century Persian mathematician**

Q: What is GCD?

Brief History of Algorithms

300 B.C.
- Euclid's gcd algorithm.

780-850 A.D.
- Abu Ja'far Mohammed Ben Musa al-Khwarizmi.

1424 A.D.
- π = 3.1415926535897932…

1845.
- Lamé: Euclid's algorithm takes at most $1 + \log_{\phi}(n\sqrt{5})$ steps.

1900.
- Hilbert's 10th problem.

1910.
- Pocklington: bit complexity.

1920-1936.
- Post, Goëdel, Church, Turing.

1965.
- Edmonds: polynomial vs. exponential algorithms.

1971.
- Cook's Theorem, Karp reductions.

20xx.
- $P \neq NP$???

Top 10 Algorithms of 20th Century

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"the greatest influence on the development and practice of science and engineering in the 20th century"

"For me, great algorithms are the poetry of computation. Just like verse, they can be terse, allusive, dense, and even mysterious. But once unlocked, they cast a brilliant new light on some aspect of computing."

-Francis Sullivan

Top 10 Algorithms of 20th Century

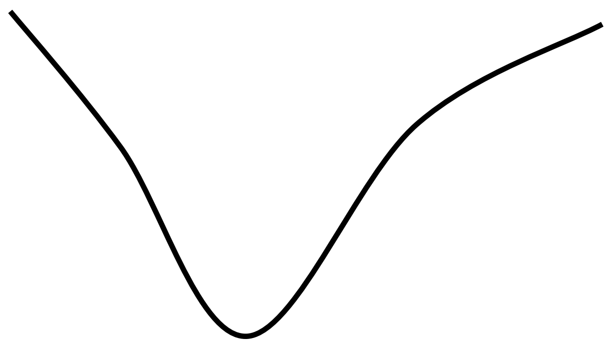
1. Metropolis Algorithm/ Monte Carlo method (Francis Sullivan, Neumann, Ulam, Metropolis, 1946). Through the use of random processes, this algorithm offers an efficient way to stumble toward answers to problems that are too complicated to solve exactly. Indeed Monte Carlo method is the only practical choice for evaluating problems of high dimensions.
   - Approximate solutions to numerical problems with too many degrees of freedom.
   - Approximate solutions to combinatorial optimization problems.
   - Generation of random numbers.

Metropolis Algorithm

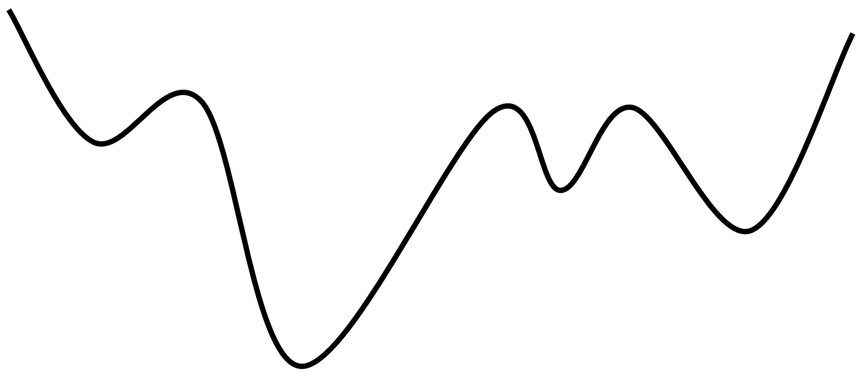
Local search. Algorithm that explores the space of possible solutions in sequential fashion, moving in one step from a current solution to a "nearby" one.

- TSP: given a tour, perturb it by exchanging order of two cities.
- VERTEX-COVER: given a vertex cover, perturb it by adding or deleting a node, so that resulting set remains a cover.

Gradient descent. Replace current solution with neighboring solution that improves objective function, until no such neighbor exists.



A funnel



A jagged funnel

Metropolis Algorithm

Simulated annealing.

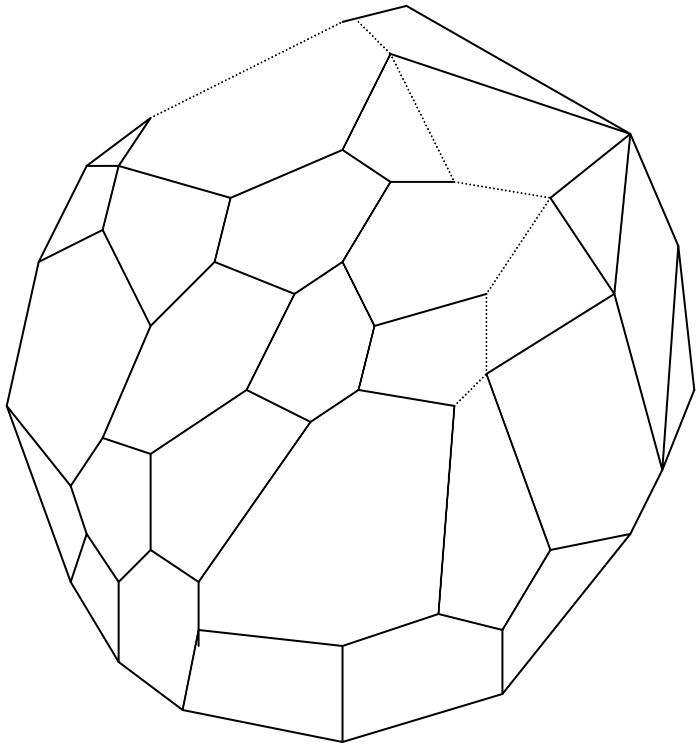
- T large $\Rightarrow$ probability of accepting an uphill move is large.
- T small $\Rightarrow$ uphill moves are almost never accepted.
- Idea: turn knob to control T.
- Cooling schedule: $T = T(i)$ at iteration i.

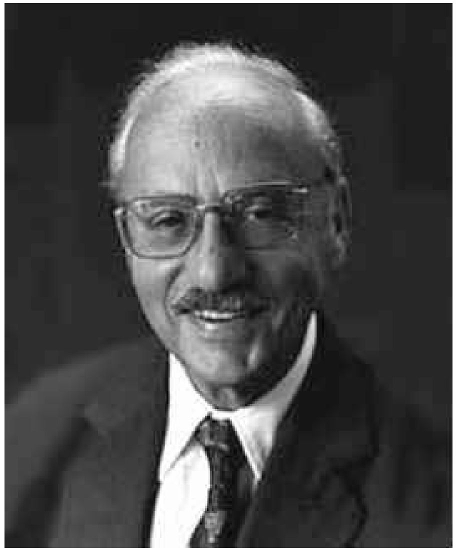
Physical analog.

- Take solid and raise it to high temperature, we do not expect it to maintain a nice crystal structure.
- Take a molten solid and freeze it very abruptly, we do not expect to get a perfect crystal either.
- Annealing: cool material gradually from high temperature, allowing it to reach equilibrium at succession of intermediate lower temperatures.

Top 10 Algorithms of 20^{th} Century

2. **Simplex Method for Linear Programming (Dantzig 1947).** An elegant solution to a common problem in planning and decision-making: $\max \{cx : Ax \le b, x \ge 0\}$.
   - One of most successful algorithms of all time.
   - Dominates world of industry.





Top 10 Algorithms of 20th Century

3. Krylov Subspace Iteration Method (Hestenes, Stiefel, Lanczos, 1950).
A technique for rapidly solving $Ax = b$ where A is a huge $n \times n$ matrix.

Subspace Iteration Method

```
Compute r(0) = b – Ax(0) for some initial guess x(0)
for i = 1,2,…
   Solve Mz(i-1)= r(i-1)
   ρ_{i-1} = r(i-1)T z(i-1)
   if i = 1
      p(1) = z(0)
   else
      β_{i-1} = ρ_{i-1}/ ρ_{i-2}
      p(i) = z(i-1) + β_{i-1} p(i-1)
   endif
   q(i) = Ap(i)
   α_i  = ρ_{i-1}/p(i)T q(i)
   x(i) = x(i-1) + α_i p(i)
   r(i) = r(i-1) - α_i q(i)
   Check convergence; continue if necessary
end
```

Preconditioned Conjugate Gradient

Top 10 Algorithms of 20th Century

4. **Decompositional Approach to Matrix Computations (Householder, 1951). A suite of technique for numerical linear algebra that led to efficient matrix packages.**
   - **Factor matrices into triangular, diagonal, orthogonal, tri-diagonal, and other forms.**
   - **Analysis of rounding errors.**
   - **Applications to least squares, eigenvalues, solving systems of linear equations.**
   - **LINPACK, EISPACK.**

Top 10 Algorithms of 20th Century

5. Fortran Optimizing Compiler (John Warner Backus, 1957). Turns high-level code into efficient computer-readable code.
   - Among single most important events in history of computing: scientists could program computer without learning assembly.
   - the inventor for the popular metalanguage BNF
   - He is the 1977 recipient of the ACM Turing Award

Fortran Code

```
500   C = 0.0
C   *** START LOOP ***
      DO 540 I=L,K
         F = S*RV1(I)
         RV1(I) = C*RV1(I)
         IF (ABS(F).LE.EPS) GO TO 550
         G = W(I)
         H = SQRT(F*F+G*G)
         W(I) = H
         C = G/H
         S = -F/H
510   CONTINUE
```

Top 10 Algorithms of 20th Century

6. QR Algorithm for Computing Eigenvalues (Francis 1959). Another crucial matrix operation made swift and practical.
   - Eigenvalues are arguably most important numbers associated with matrices.
   - Differential equations, population growth, building bridges, quantum mechanics, Markov chains, web search, graph theory.

$$\boxed{A x = \lambda x}$$

QR(A)

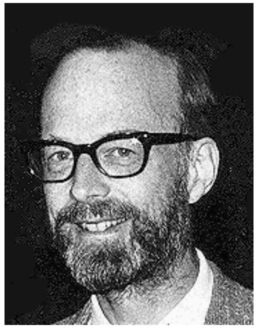
```
Initialize A0 = A

FOR k = 0, 1, 2, ...
   Factor  Ak   = Qk Rk
   Compute Ak+1 = Rk Qk
```

$$A_{k+1} = R_k Q_k$$
$$= Q^{-1}{}_k Q_k R_k Q_k$$
$$= Q^{-1}{}_k A_k Q_k$$
$$\Rightarrow A_{k+1} \text{ and } A_k \text{ have same eigenvalues}$$

Top 10 Algorithms of 20th Century

7. **Quicksort (Hoare, 1962). Given n items over a totally order universe, rearrange them in increasing order.**
   - $O(n \log n)$ **instead of** $O(n^2)$.
     - » **Efficient handling of large databases.**
   - **He is the 1980 recipient of the ACM Turing Award**
     - » **For his fundamental contributions to the definition and design of programming languages.**

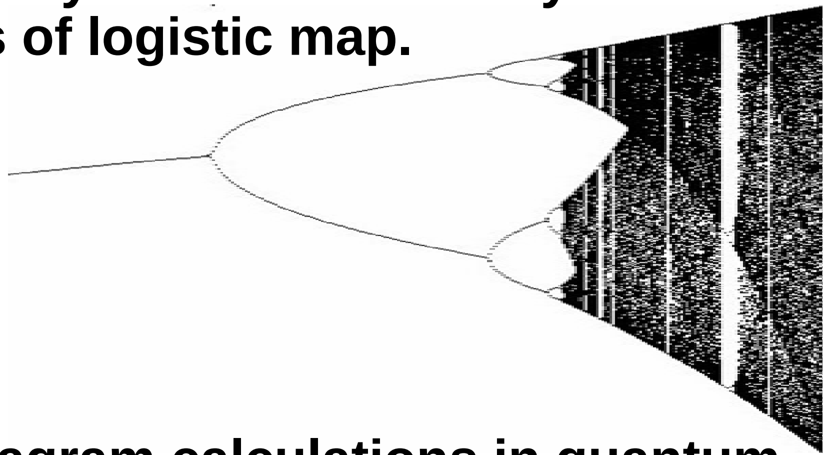


8. **Fast Fourier Transform (Cooley, Tukey 1965). Perhaps the most ubiquitous algorithm in use today, it breaks down waveforms (like sound) into periodic components.**
   - $O(n \log n)$ **instead of** $O(n^2)$ **by Runge- König (1924).**
     - » **foundation of signal processing**
     - » **CD players, JPEG, analyzing astronomical data, etc.**

Top 10 Algorithms of 20^{th} Century

9. **Integer Relation Detection (Ferguson, Forcade, 1977).**
   Given real numbers $x_1, \ldots, x_n$, find integers $a_1, \ldots, a_n$ (not all 0 if they exist) such that $a_1x_1 + \ldots + a_nx_n = 0$?
   - **PSLQ algorithm generalizes Euclid's algorithm: special case when $n = 2$.**
   - **Find coefficients of polynomial satisfied by 3^{rd} and 4^{th} bifurcation points of logistic map.**

$$x_{n+1} = ax_n(1 - x_n)$$

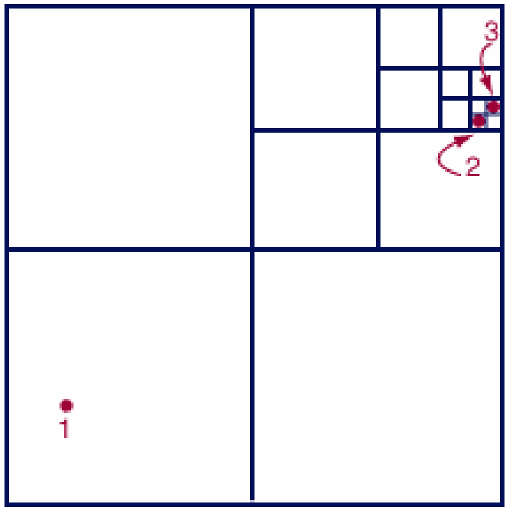


   - **Simplify Feynman diagram calculations in quantum field theory.**
   - **Compute nth bit of π without computing previous bits.**
   - **Experimental mathematics.**

Top 10 Algorithms of 20th Century

10. Fast Multipole Method (Paul Greengard, Rokhlin, 1987). Accurate calculations of the motions of *n* particles interacting via gravitational or electrostatic forces.

- **Central problem in computational physics.**
- **$O(n)$ instead of $O(n^2)$.**
- **Celestial mechanics, protein folding, etc.**



A Quad-Tree